Update to and Recent Performance of the NAM-CMAQ Air Quality Forecast Model at NCEP operations

Jeff McQueen*, Pius Lee, Marina Tsidulko, Geoff DiMego
Mesoscale Modeling Branch
NOAA/NWS/NCEP/Environmental Modeling Center

Rohit Mathur, Tanya Otte, Jon Pleim, George Pouliot, Jeff Young and Daiwen Kang
NOAA/ARL/Atmospheric Sciences Modeling Division
(On assignment to the EPA/National Exposure Research Laboratory)

Paula Davidson and Nelson Seaman
NOAA/NWS/Office of Science and Technology

1. INTRODUCTION

NOAA and EPA have developed and operationally implemented a new ozone forecast capability, in response to Congressional direction (Davidson et al. 2004). This capability builds on decades of research collaboration, culminating in a NOAA-EPA MOA for air quality forecasting, signed in 2003. The NWS/ National Centers for Environmental Prediction (NCEP) Eta model at 12 km was used to provide meteorological predictions for the EPA Community Multi-scale Air Quality (CMAQ) model to produce 48 h ozone predictions. The CMAQ system simulates various chemical and physical processes that are important for modeling atmospheric trace gas transformations and distributions. Initial description and evaluation of the Eta-CMAQ forecast system was described by Otte, et al. (2004).

This paper describes the improvements to and performance of the NOAA Eta-CMAQ modeling system that were run at the NWS/NCEP operational computer center for real-time air quality forecasting. In the Summer 2004, two systems were tested and evaluated; a now Operational NE U.S. domain run and a now experimental Eastern U.S domain run.

In 2005, a developmental CONUS domain run was added for evaluation by a focus group of State air quality forecasters. The operational and experimental systems are run twice per day at 12 km resolution at 06 and 12 UTC with forecasts to 48 hours. The system was run with updates to the both the Eta-12 and CMAQ modeling systems including 6 hour cycling for initial CMAQ conditions, use of the NCEP Global Forecast System(GFS) ozone predictions (Lee, et al, 2004) to prescribe CMAQ upper lateral boundary conditions, and updates to the CMAQ model convective and PBL mixing and emissions. These predictions were configured with CMAQ gas-phase chemistry only, however, daily 24h forecast research runs are made over the Eastern U.S. with aerosols turned on.

Specifically, this paper will overview the operational and experimental system implemented including the NCEP-Eta weather model fields used drive CMAQ. The NCEP Forecast Verification Systems (FVS) and NWS/MDL verification systems were used to summarize general model performance and biases as compared to the EPA AIRNOW observational network.

2. 2004 NOAA-EPA AQ PREDICTION SYSTEM

Beginning in the Summer 2004, NCEP added a coupled Eta-CMAQ air quality prediction system to provide 48 h predictions of surface ozone for the Eastern U.S. In 2005, an expanded grid developmental run covering the Continental U.S. is undergoin testing (See Table 3).

The operational NE U.S. domain and experimental expanded domains are shown in Fig. 1. All systems consisted of the following components:

- .*The NCEP/EMC North American Eta 12 km 60 level prediction system* for gridded meteorological model predictions at hourly intervals. (Rogers et al. 1996). Recent improvements to the Eta system are described by Ferrier et al. (2003). These changes included improved grid-scale cloud microphysics and interactions with short

*Corresponding Author Address: Jeff McQueen, NCEP/EMC, W/NP22 Room 207, 5200 Auth Road, Camp Springs, MD 20746-4304; jeff.mcqueen@noaa.gov

and long-wave radiation. Direct analysis of the WSR-88D radar radial velocities and use of NOAA-17 satellite radiances were incorporated into the EDAS 3DVAR assimilation system.

- *The modified Eta product generator,* interpolates Eta native grid model outputs (rotated lat-lon Arakawa E grid) to an intermediate grid with 22 terrain-following sigma vertical layers. (Table 1).
- *The CMAQ preprocessor, PREMAQ,* prepares the CMAQ-ready meteorological and emissions files. Table 2 summarizes the PREMAQ configuration used for the summer 2004.
- *The CMAQ atmospheric chemistry model* (Byun and Ching, 1999) provides the ozone forecasts. The CMAQ configuration is described in Table 3. In 2004, a minimum limit was set on PBL mixing of chemistry to improve over-predictions in rural areas. In 2005, downward entrainment of high ozone air above deep convective clouds was eliminated to help remove overprediction biases seen in 2004. For the CONUS tests, an alternative convective cloud mixing scheme is undergoing testing and photolysis is scaled by the NAM clear sky radiation predictions.
- *Boundary conditions*: For the summer 2004 and 2005, the NCEP Global Forecast System (GFS) ozone predictions were used above 6 km (Lee, et al, 2004). Below 6 km, a climatological chemical profile was assumed for the lateral boundary conditions, which were kept constant with time. For the CONUS run, tests are being performed with the use of GFS ozone for CMAQ lateral boundaries at the CMAQ model top layer only.
- *Initial Conditions*: A 6-hour cycling system was developed and run 4 times per day to initialize CMAQ chemistry and soil fields to reduce spinup of soil and chemical constituents. (McQueen, et al*., 2004)*

Table 1. Fields added to the Eta post-processor to couple with CMAQ. Fields are output hourly and on the CMAQ sigma layers.

Eta Variable name	**Used for CMAQ:**
Geopotential height	*Transport*
Pressure	*Transport*
Temperature	*Biogenics, vertical mixing*
Specific humidity	*Cloud processes, photolysis*
U & V winds	*Transport*
Vertical velocity	*transport*
Canopy conductance	Air-sfc exchange
PBL height	Vertical mixing
Plant canopy water	Air-sfc exchange
Vertical Eddy Heat diffusivity	Tested w/ mixing

3. FORECAST PRODUCTS

Predictions of ground-level ozone concentration were made twice each day driven by the 0600 and 1200 UTC Eta forecast cycles. Both 0600 and 1200 UTC CMAQ forecasts were run to 48 h.

The CMAQ system was run on the NCEP IBM SP super-computer using 33 (NE 1x domain) or 65 processors (East 3x domain). 48 hour CMAQ forecasts required 45 minutes of cpu time for the NE domain. The 0600 and 1200 UTC model guidance was required to be available on the NWS Telecommunications Operations Center server by 1730 UTC, while the 0600 UTC 48 hour guidance was required by 1300 UTC.

Predicted 1-hour and 8 hour average surface ozone concentrations were output on the CMAQ grid in WMO GRiB format for further visualization and evaluation against the data provided by EPA's AIRNOW surface ozone measurement network (Wayland, et al., 2002). Additional fields were also output and several levels plotted for the NE and Eastern U.S. Domain. These included the following at 19, 65, 350 and 1250 m AGL: NOx, NOy, NO, NO2, Formaldehyde, and CO. Several meteorological predicted parameters were also produced including cloud cover, incoming radiation, PBL heights and ventilation index. Examples of ozone forecasts on both the NE (1x) and expanded Eastern U.S. (3x) domains are shown in Figure 1.

Table 2. PREMAQ Emission Configuration	
Point Sources	Pre-computed (updated for 2005) temporal emissions factors with met. Dependent plume rise effects calculated each hour.
Area	Pre-computed (updated for 2005) for each day of year.
Mobile	Pre-computed emission factors from MOBILE 6 with hourly temperature-dependent effects.

Biogenic	BEIS-3, using Eta temperature and radiation variables (Pierce et al. 2002)

4. SUMMER 2004 SYSTEM EVALUATION

Statistical evaluation for June–Sept, 2004 for ozone monitors in each of the CMAQ domains was performed with the NCEP FVS and NWS MDL verification systems. Both systems performed standard statistics (RMSE, Bias, etc) and contingency statistics (accuracies, Probability of detection, skill scores). FVS Examples are shown in Fig. 2 for the 1200 UTC cycle prediction. Additional evaluations are shown at: http://wwwt.em.ncep.noaa.gov/mmb/aq/ The RMSE and biases (not shown) for 1-h average predictions all indicate an over prediction of ozone with errors highest during the night time hours. For both grids, larger errors were found over the NE US as compared to the SE sub- region. In general, the expanded 3x CMAQ domain forecasts over the NE 1x domain show slightly larger errors as compared to the 1x domain forecasts. The cause of the larger errors over the 3x domain was partially overcome by modifying the CMAQ convective cloud mixing scheme.

Eta predictions were also evaluated for the Northeastern U.S. during the Summer 2004 NE High Resolution Temperature program. Boundary layer profilers and surface radiation budget stations deployed were used to further diagnose errors in the Eta-CMAQ prediction system. During the Summer 2004, Eta surface temperature predictions were slightly warmer than observed in the daytime in the NE (Fig. 3). Incoming solar insolation (Fig. 4) was slightly over-predicted on average by as much as 50-100 W/m2 as represented by the Pennsylvania State University solar radiation observation site. For the 2004 AQ system, over predicted solar insolation would affect only the biogenic emissions because predicted photolysis rates were affected primarily by cloud coverage, derived from Eta forecasted RH.

5. 2005 SENSITIVITY TESTS

Several sensitivity experiments were performed for the Eastern U.S. domain to fully evaluate possible modifications. Retrospective testing were performed by NOAA/OAR and EPA for the following periods:

- 12Z July 16, 2004 – 12Z July 25, 2004
- 12Z August 4, 2004 – 12Z August 13, 2004
- 12Z August 8, 2002 – 12Z August 20, 2002

The following sensitivity experiments were performed:

- 2004 Base: 2004 Eastern U.S. run
- **S0:** Reflects changes due to Eta-X
- **S1**: S0 + photolysis attenuation based on Eta radiation fields
- **S3**: S0 + Mixing from above clouds turned-off
- **S5**: S1+S3

The results of these sensitivity experiments for the July 2004 episode are shown in Fig. 6. Correlations coefficients and biases are generally improved for the S3 and S5 tests. During hot and humid, clear-sky conditions when high ozone was observed (generally observed from July 17-20 in the Eastern U.S.), improvements in the S3 and S5 runs were largest. The effect of using NAM clear sky radiation values to scale CMAQ photolysis rates (SO) was minimal. This change was not implemented at this time into the experimental Eastern U.S. runs.

6. SUMMARY

This paper summarized an experimental air quality prediction system that coupled the NWS operational NAM-12 meteorological model with the CMAQ model to produce twice-daily ozone guidance. Care was taken in coupling the two models to reduce interpolation errors caused by converting NAM Eta meteorological fields to the CMAQ grids. In addition, CMAQ was optimized to run efficiently in a forecast mode.

Over prediction of ozone was reduced from 2003 and 2004 results in most areas. Some of this error was corrected by modifying the CMAQ convective cloud mixing. Future upgrades include driving CMAQ with the Weather Research and Forecast (WRF) meteorological model, improved coupling with the NAM boundary layer, cloud and radiation parameter predictions, improving CMAQ chemical boundary conditions and further testing with aerosols.

ACKNOWLEDGEMENTS

Thanks to the EPA AIRNOW program for providing surface based ozone measurements used for model evaluation**.** The views expressed are those of the authors and do not necessarily represent those of NOAA or the EPA.

REFERENCES

Byun, D. W., and J. K. S. Ching (Eds.), 1999: Science algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System. EPA-600/R-99/030, Office of Research and Development, U.S. Environmental Protection Agency, Washington, D.C. [Available from U.S. EPA, ORD, Washington, D.C. 20460.]

Davidson, P.M., N. Seaman, K. Schere, R.A. Wayland, J.L. Hayes and K.F. Carey, 2004: National Air Quality Forecasting Capability: First Steps toward Implementation. Preprints, 6th Conference on Atmospheric Chemistry: Air Quality in Megacities. Seattle, WA, Jan 11-15, 2004.

Ferrier, B., Y. Lin, D. Parrish, M. Pondeca, E. Rogers, G. Manikin, M. Ek, M. Hart, G. DiMego, K. Mitchell, and H. Chuang, 2003: Changes to the NCEP Meso Eta Analysis and Forecast System: Modified cloud microphysics, assimilation of GOES cloud-top pressure, assimilation of NEXRAD 88D radial wind velocity data. [Available at http://wwwt.emc.ncep.noaa.gov/mmb/tpb.spring03/tpb.htm or from the National Weather Service, Office of Climate, Water and Weather Services, 1325 East-West Highway, Silver Spring, MD 20910].

Lee, P.C., et al., 2004: Linking the Eta Model with the CMAQ modeling system: Ozone boundary conditions. Preprints, 27th NATO/CCMS ITM on Air Pollution Modeling and its Application. Oct. 8pp.

McQueen, J.T., et al., 2004: : Development and Evaluation of the NOAA/EPA Prototype Air Quality Model Prediction System. Proceedings, Sixth Conference on Atmospheric Chemistry: Air Quality in Megacities. J2.16, Seattle, WA 10pp.

Otte, T., et al. 2005: Linking the Eta model with the Community Multiscale Air Quality (CMAQ) Modeling system to build a national air quality forecasting system. Wea. Forec., 2005,367-384.

Pierce, T., C. Geron, G. Pouliot, E. Kinnee, and J. Vukovich, 2002: Integration of the Biogenic Emissions Inventory System(BEIS3) into the Community Multiscale Air Quality Modeling System. Preprints, 12th Joint Conf. on the Apps. of Air Pollu. Meteor. with the A&WMA, Amer. Meteor. Soc., Norfolk VA, 20-24 May 2002, J85-J86.

Rogers, E., T. Black, D. Deaven, G. DiMego, Q. Zhao, M. Baldwin, N. Junker, and Y. Lin, 1996: Changes to the operational "early" Eta Analysis/Forecast System at the National Centers for Environmental Prediction. Wea. Forecasting, 11, 391-413.

Wayland, R. A., J. E. White, P. G. Dickerson, and T. S. Dye, 2002: Communicating real-time and forecasted air quality to the public. Environ. Manage., December, 28-36.

Table 3. 2004/2005 CMAQ NE and Expanded Grids Configuration				
(began-)	NE U.S. (5/1/04-)	East U.S. (6/1/04-)	Aerosols (7/16/04 -)	CONUS (6/1/05 -)
Grid	Lambert-Conformal Arakawa C Centered at 40.5N, 79.5W and true at 36N and 46N.	Lambert-Conformal Arakawa C true at 33N and 45N.	Lambert-Conformal Arakawa C true at 33N and 45N.	Lambert-Conformal Arakawa C
Nx,Ny	166x142	268x259	268x259	469x256
Grid Spacing	12 km, lower-left corner at: (32.353N, 89.994W)	12 km, lower-left corner at:(24.595N, 100.99W)	12 km:lower-left corner at:(24.595N, 100.99W)	12 km, 22 levels
Runs/day	06Z, 12 Z out to 48hrs	06Z, 12 Z out to 48 hrs	12Z out to 24 hours	12Z out to 48 hours
Run-time/12z availability	45 mins/15:30 UTC	2 hrs/ 16:30 UTC	6 hrs/ 21:00 UTC	~3 hrs/18:00 UTC

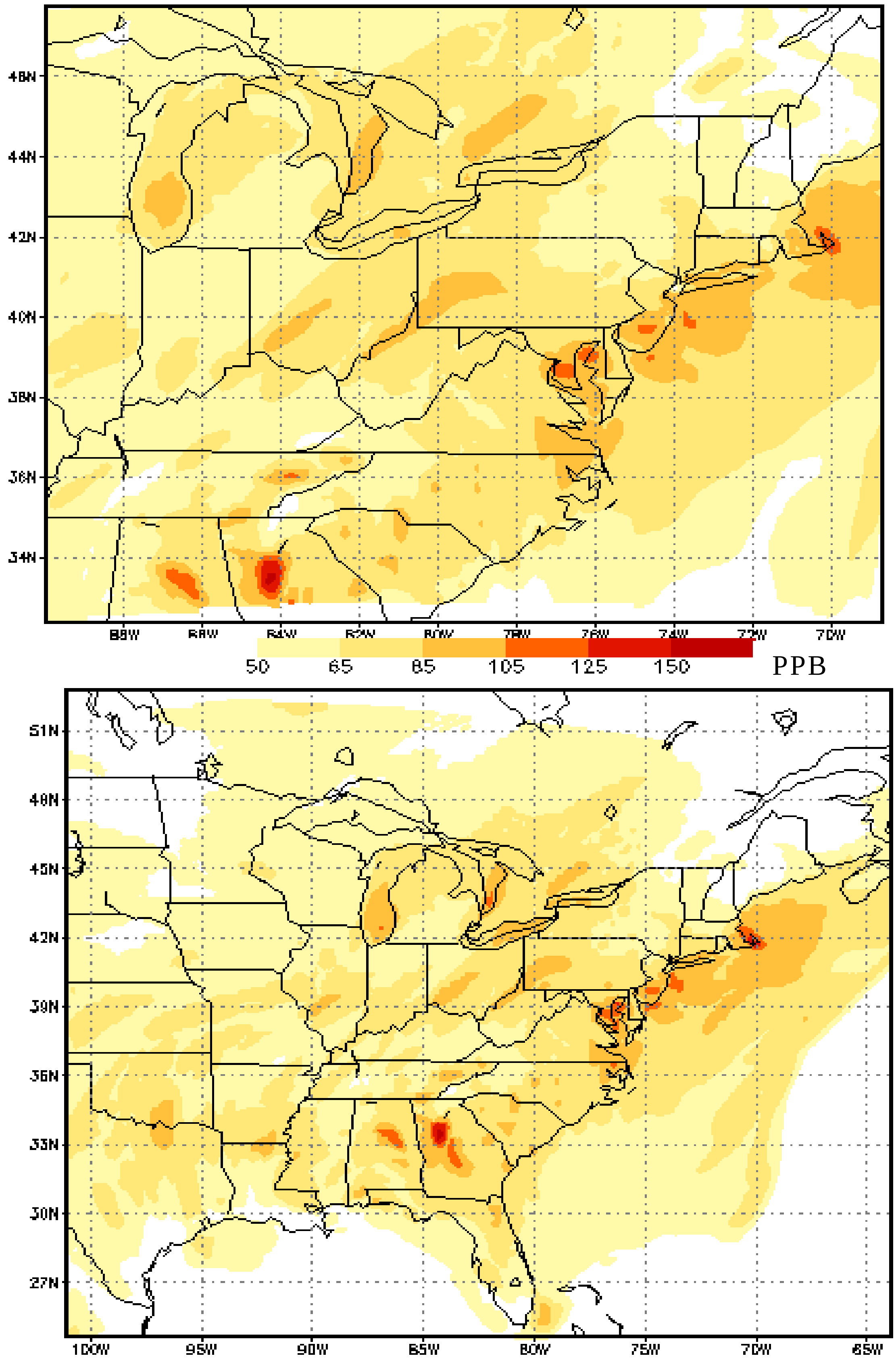

Figure 1. Example of ozone predictions for July 21, 2004. A) Day 1 max imum O3 (ppb) on the NE grid (CMAQ 1x) and B) Eastern US grid (CMAQ 3x).

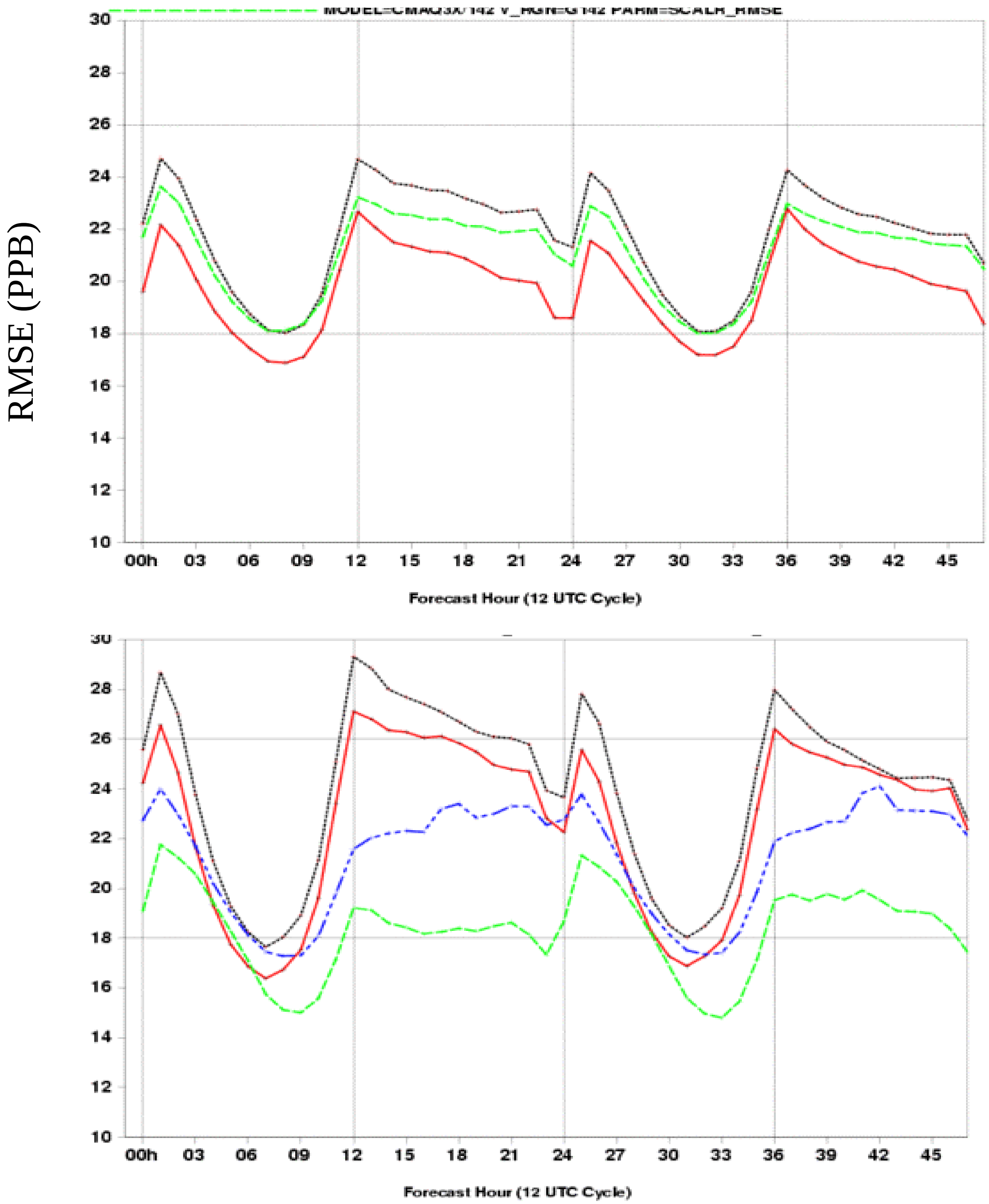

Figure 2. Mean predicted CMAQ ozone concentration errors in ppb for August 2004 A) Root Mean Square error (red: CMAQ 1x. Black: CMAQ 3x errors only over 1x domain, Green: CMAQ 3X whole domain) B) Sub-regional RMSE over the NE sub-region for the CMAQ 1x (red) and CMAQ 3x (black) forecasts and the SE sub-region for the CMAQ 1x (green) and CMAQ 3x (blue) forecasts.

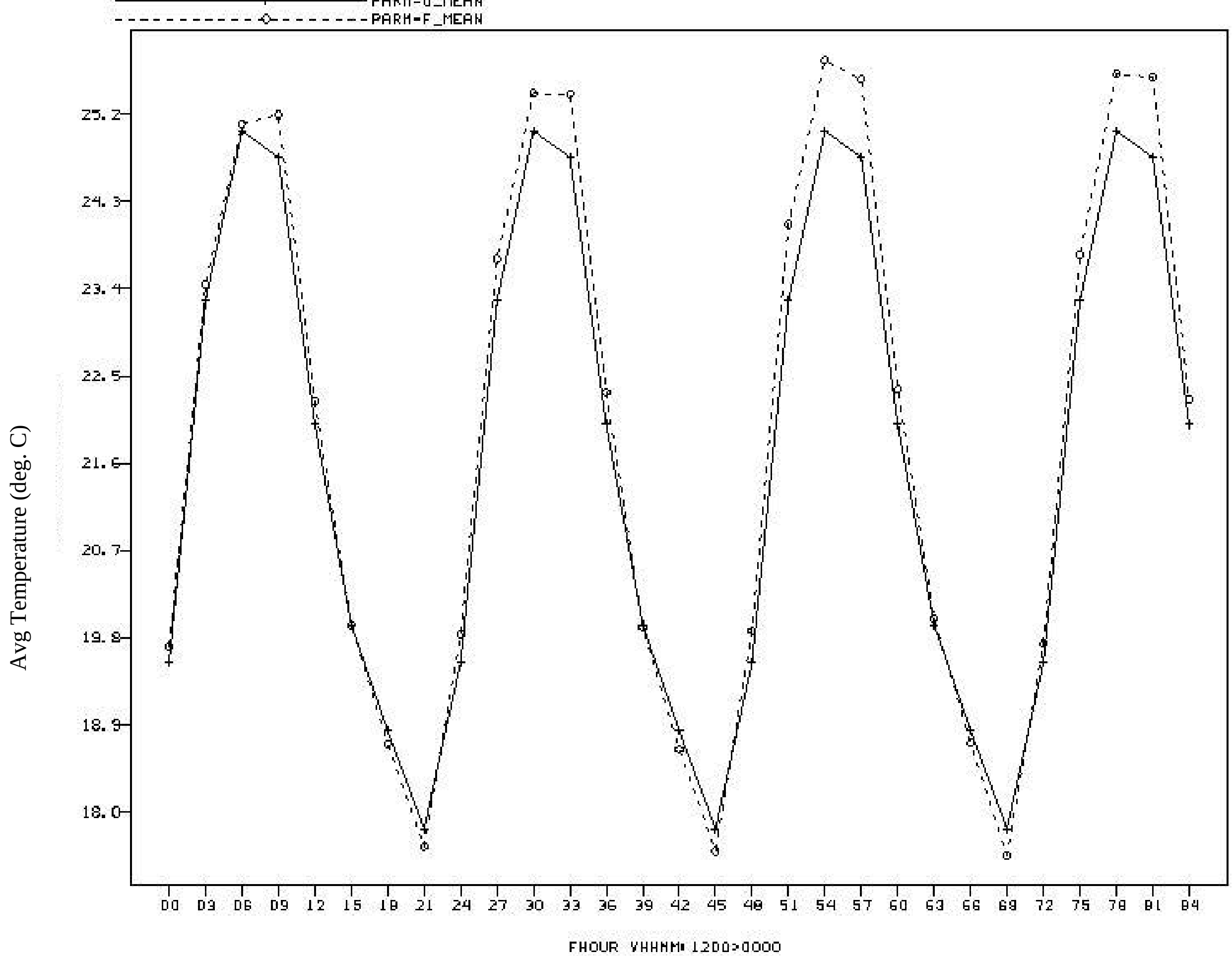

Figure 3. Mean errors from the Eta forecast 12 UTC cycle during August 2004 of 2 m temperature averaged by forecast hour over the NE region (deg. C) , observed(solid line) Eta (dashed).

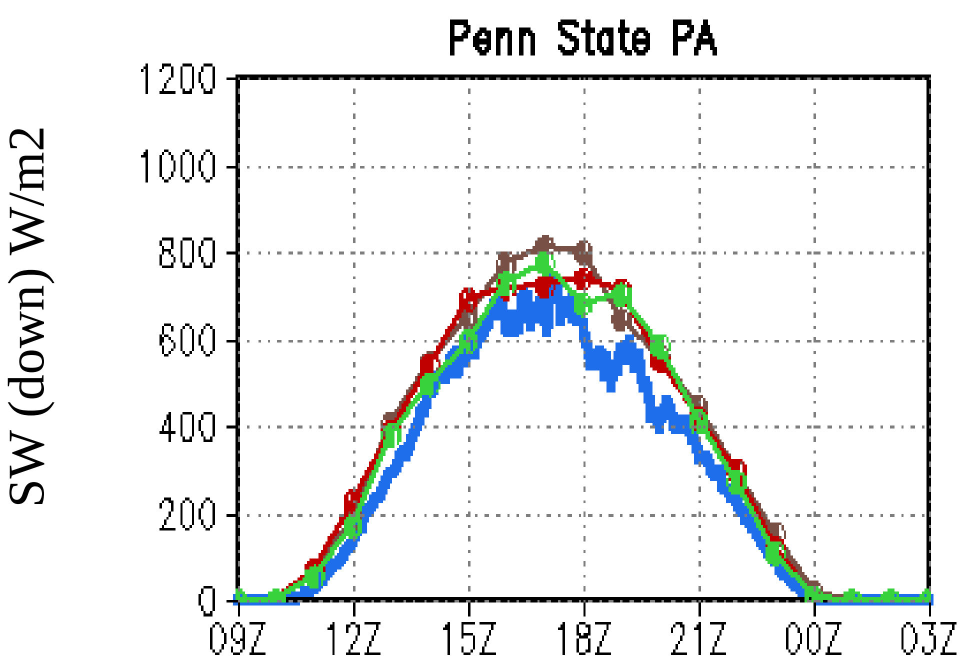

Figure 4. Mean errors from the Eta forecast 12 UTC cycle during August 2004 of Incoming short wave heat fluxes averaged by UTC hour (W/m^2 , observed(blue), Eta forecast(red), Experimental Eta forecast w/ GFS radiation scheme (green) and the Eta Data Assimilation System (EDAS, brown).

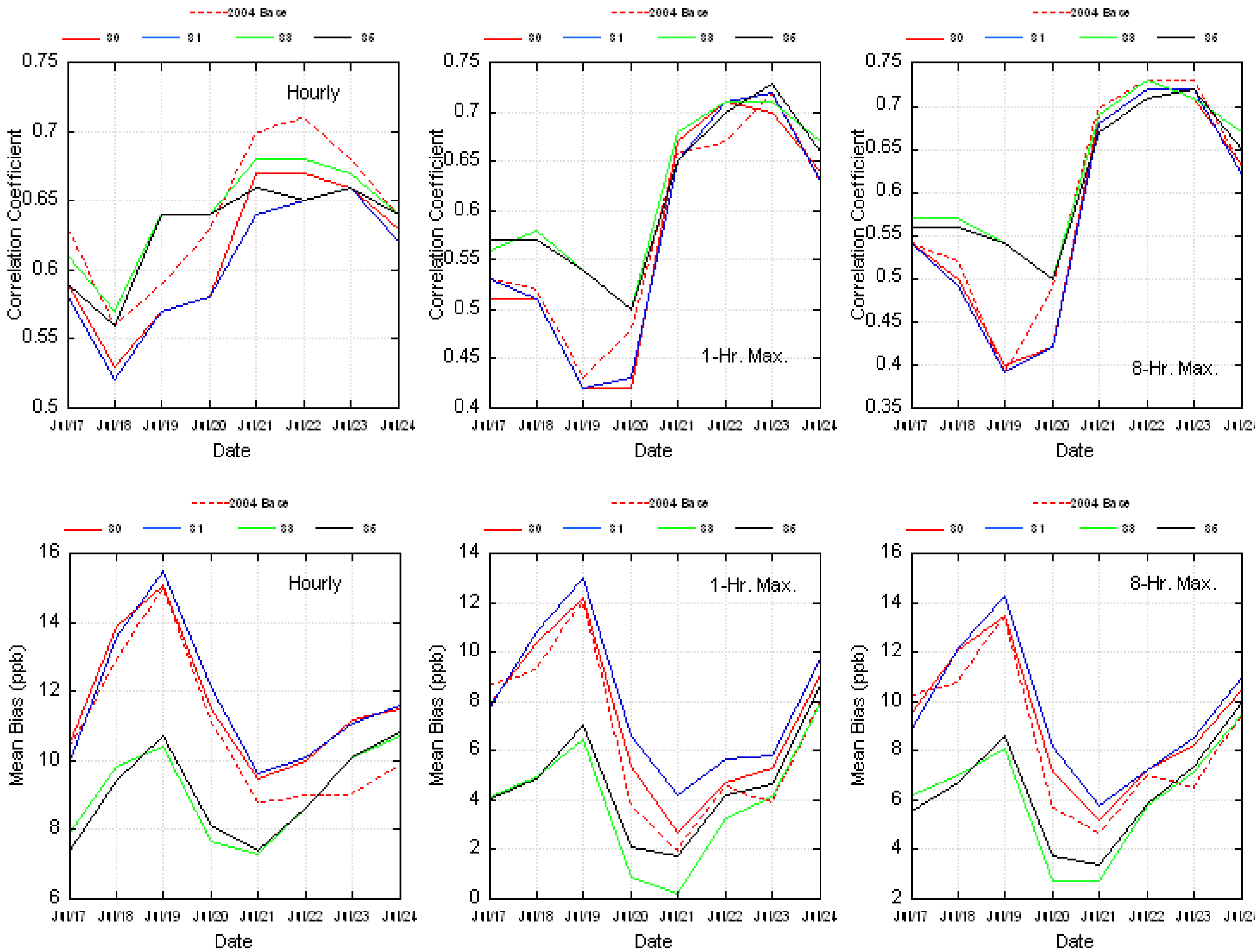

Figure 6. Evaluation of various NAM-CMAQ configurations tested for the Summer 2005. Hourly averaged, 1-hr and 8 hr max predictions correlation coefficiants and mean biases computed against AIRNOW surface